MS30-O3 **Twin samples with CrysAlisPro: Experiments, unit cell finding, data reduction and post corrections.** Mathias Meyer, *Agilent Technologies (Poland) Sp. z o.o., Szarskiego 3, PL-54-610 Wroclaw*
E-mail: Mathias.Meyer@agilent.com

Crystallographers usually scrutinize their sample selection process to avoid twinned or multi-crystal samples to get the best possible data. But some samples will only reveal themselves as twins (non-merohedric) during the diffraction experiment.

This talk will focus on the tools implemented in Agilent's XRD experiment and data reduction work bench 'CrysAlisPro' to deal with twinned samples at various stages of the experiment:

- Twin detection in pre-experiment data
- EwaldPro: a new tool for reciprocal space investigations and easy twin detection
- Challenges in twin unit cell finding: 'easy twins' and 'super-lattice fakers'.
- Data collection strategy with known twin law.
- Data reduction of twin data.
- Scaling and empirical correction for twin data
- Shape description and numerical absorption correction for twin samples
- Boot strap the structure solution process for twin samples (multi-HKLF4 files, data rejection)
- Use of AutoChem with twins
- Optimal use of HKLF4 and 5 format for structure refinement

With the offered tool set within 'CrysAlisPro' twin handling is straightforward and easy to grasp also for non-expert users.

Keywords: Area detector; data reduction; twin

MS30-O4 **Oligo-diffractometry using EVAL15.** Martin Lutz, Loes M. J. Kroon-Batenburg, *Utrecht University, Bijvoet Center for Biomolecular Research, Crystal and Structural Chemistry, Padualaan 8, 3584CH Utrecht, The Netherlands*
E-mail: m.lutz@uu.nl

The term oligo-diffractometry describes the phenomenon that a crystal is composed of several phases [1]. As an example, we present an organometallic titanium complex which consisted of two phases, $[C_{20}H_{17}Cl_4N_4Ti] \cdot C_7H_8$ with a unit cell volume of 2794.9(2) $Å^3$ and $[C_{20}H_{17}Cl_4N_4Ti]$ with a volume of 2276.3(4) $Å^3$. Indexing of the two unit cells was performed semi-automatically using Dirax [2]. Both phases have a monoclinic P-cell with similar values for a, b, and β. The lengths of the c-axes are different (26.8233(16) *vs.* 21.190(3) Å). Intensity data were measured on a Bruker Kappa ApexII diffractometer with Mo-radiation, a detector distance of 55 mm and a rotation angle of 0.5°. The Eval15 software [3] was used for the integration of the data using predicted *ab initio* profiles. Intensities of neighboring/overlapping reflections were obtained with singular value decomposition. Main reflection and neighboring reflections are deconvoluted, if the covariance between these reflections is smaller than 0.02*variance(main). All other reflections were considered as overlapping and consequently summed. For the major crystal component (toluene solvate) a completeness of 77 % was achieved, and for the minor component (solvent free) the completeness was 70 %. This completeness was sufficient for structure solution and refinement with SHELX [4]. Subsequently, the overlapping reflections can be split based on F^2_{calc}.

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Keywords: indexing; intensity measurement; diffraction profile simulation